Exact Solutions of Schrödinger Equation for a Ring-Shaped Potential

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Abstract

The exact solutions of Schrödinger equation are obtained for a noncentral potential which is a ring-shaped potential. The energy eigenvalues and corresponding eigenfunctions are obtained for any angular momentum ℓ. Nikiforov-Uvarov method is used in the computations.

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1 Introduction

Exact solutions of the fundamental wave equations of the non-relativistic quantum mechanics have attracted much attention in recent years. So far many efforts have been made to solve the time-independent Schrödinger equation for non-central potentials in three and two dimensions such as the Coulombic ring-shaped potential [1-5] and deformed ring-shaped potential [6], the Hellmann potential [7]. In quantum mechanics, Aharonov-Bohm (AB) effect is an another popular non-central potential type [8]. It is also studied through the wide areas such as path integral solutions[9], in non-commutative quantum mechanics [10], a Dirac particle in the Aharonov-Bohm potential [11-13] and scattering [14]. On the other hand, AB potential is also known as ring shape potential [6].

Recently, an alternative and simple method called as Nikiforov-Uvarov Method [15] (NU-method) has been introduced for solving the Schrödinger equation for some well known potentials [16-18]. It is also used to solve the Klein-Gordon and Duffin-Kemmer-Petiau wave equations in the presence of exponential type potentials such as standard Woods-Saxon [19], Pöschl-Teller [20] and Hulthen potentials [21-23]. The Nikiforov-Uvarov method [15] is used in the computations to obtain energy eigenvalues and the corresponding eigenfunctions. Recently Alhaidari et al have studied Dirac and Klein Gordon equation for the Coulomb, oscillator and Hartmann potentials [24].

Ring shaped potential has an application field in quantum chemistry as a model for the Benzene molecule given as [1,4,9]

$$V_q(r) = \eta \sigma^2 \epsilon_0 \left(\frac{2a_0}{r} - \frac{\eta a_0^2}{r^2 sin^2 \theta} \right) \tag{1}$$

where $a_0 = \frac{\hbar^2}{\mu e^2}$, $\epsilon_0 = -\frac{1}{2} \frac{\mu e^4}{\hbar^2}$, Bohr radius and the ground state energy of the hydrogen atom, respectively, μ is the particle mass, η and σ are dimensionless positive real parameters which range from about 1 to 10 [9].

The paper is arranged as follows. In section II, the Nikiforov-Uvarov Method is given briefly. In section III, NU method is applied to three dimensional Schrödinger equation with the ring shaped potential. Results are discussed in section IV.

2 The Nikiforov-Uvarov Method

The NU-method developed by Nikiforov and Uvarov is based on reducing the second order differential equations (ODEs) to a generalized equation of hypergeometric type [15]. It is provided us an analytic solution of Schrödinger equation for certain kind of potentials. This is based on the solutions of general second order linear differential equation with orthogonal functions [15]. For a given appropriate potential, the one-dimensional Schrödinger equation is reduced to a generalized equation of hypergeometric type with a suitable coordinate transformation $s = s(r)$. Then, the equation has the form,

$$\psi^{''}(s) + \frac{\tilde{\tau}(s)}{\sigma(s)}\psi^{'}(s) + \frac{\tilde{\sigma}(s)}{\sigma^2(s)}\psi(s) = 0 \tag{2}$$

where $A(s) = \frac{\tilde{\tau}(s)}{\sigma(s)}$ and $B(s) = \frac{\tilde{\sigma}(s)}{\sigma^2(s)}$. In Eq.(2), $\sigma(s)$ and $\tilde{\sigma}(s)$ are polynomials at most second degree. $\tilde{\tau}(s)$ is a polynomial with at most first degree [15]. The wave function is constructed as a multiple of two independent parts,

$$\psi(s) = \phi(s)y(s), \tag{3}$$

and Eq.(2) becomes [15]

$$\sigma(s)y^{''}(s) + \tau(s)y^{'}(s) + \lambda y(s) = 0, \tag{4}$$

where

$$\sigma(s) = \pi(s)\frac{d}{ds}(ln\phi(s)), \tag{5}$$

and

$$\tau(s) = \tilde{\tau}(s) + 2\pi(s). \tag{6}$$

λ is defined as

$$\lambda_n + n\tau^{'} + \frac{[n(n-1)\sigma^{''}]}{2} = 0, n = 0, 1, 2, ... \tag{7}$$

determine $\pi(s)$ and λ by defining

$$k = \lambda - \pi^{'}(s). \tag{8}$$

and the function $\pi(s)$ becomes

$$\pi(s) = (\frac{\sigma' - \tilde{\tau}}{2}) \pm \sqrt{(\frac{\sigma' - \tilde{\tau}}{2})^2 - \tilde{\sigma} + k\sigma} \qquad (9)$$

The polynomial $\pi(s)$ with the parameter s and prime factors show the differentials at first degree. Since $\pi(s)$ has to be a polynomial of degree at most one, in Eq.(9) the expression under the square root must be the square of a polynomial of first degree [15]. This is possible only if its discriminant is zero. After defining k, one can obtain $\pi(s)$, $\tau(s)$,$\phi(s)$ and λ. If we look at Eq.(5) and the Rodrigues relation

$$y_n(s) = \frac{B_n}{\rho(s)} \frac{d^n}{ds^n}[\sigma^n(s)\rho(s)], \qquad (10)$$

where C_n is normalization constant and the weight function satisfy the relation as

$$\frac{d}{ds}[\sigma(s)\rho(s)] = \tau(s)\rho(s). \qquad (11)$$

where

$$\frac{\phi'(s)}{\phi(s)} = \frac{\pi(s)}{\sigma(s)}. \qquad (12)$$

3   Solutions of The Ring-Shaped Potential

Let us start with the Schrödinger equation in three dimensions written as

$$-\frac{\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right) + V(r,\theta) - E\right]\phi(r,\theta,\varphi) = 0 \quad (13)$$

where $V(r,\theta)$ is taken as below

$$V(r,\theta) = -\frac{A}{r} + \frac{B}{r^2 sin^2\theta} \qquad (14)$$

A and B parameters are used instead of the parameters defined in Eq.(1) for simplicity. If we take the spherical wave function as $\phi(r,\theta,\varphi) = R(r)Y(\theta,\varphi)$ in order to separate the Schrödinger equation into variables, we obtain

$$\frac{1}{R(r)}\frac{\partial}{\partial r}\left(r^2\frac{\partial R(r)}{\partial r}\right) + \frac{2\mu Ar}{\hbar^2} + \frac{2\mu Er^2}{\hbar^2} + \frac{1}{Y(\theta,\varphi)}\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y(\theta,\varphi)}{\partial\theta}\right) - \qquad (15)$$

$$\frac{2\mu B}{\hbar^2 sin^2\theta} + \frac{1}{Y(\theta,\varphi)}\frac{1}{sin^2\theta}\frac{\partial^2 Y(\theta,\varphi)}{\partial\varphi^2} = 0 \qquad (16)$$

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Using $Y(\theta, \varphi) = H(\theta)\Phi(\varphi)$ to separate the Schrödinger equation into variables, the following three equations are obtained as:

$$\frac{d^2R(r)}{dr^2} + \frac{2}{r}\frac{dR(r)}{dr} + \frac{2\mu}{\hbar^2}\left(E + \frac{A}{r} - \frac{\hbar^2}{2\mu}\frac{\lambda}{r^2}\right)R(r) = 0, \tag{17}$$

$$\frac{d^2H(\theta)}{d\theta^2} + cot\theta\frac{dH(\theta)}{d\theta} + \left(\lambda - \frac{m^2}{sin^2\theta} - \frac{2\mu B}{\hbar^2 sin^2\theta}\right)H(\theta) = 0, \tag{18}$$

and

$$\frac{d^2\Phi(\varphi)}{d\varphi^2} + m^2\Phi(\varphi) = 0. \tag{19}$$

where m^2 and λ are separation constants. The solution of Eq.(18) is

$$\Phi_m = Ae^{im\varphi}, \quad m = 0, \pm1, \pm2, ... \tag{20}$$

We will first solve the radial part of the Schrödinger equation. If we put $R(r) = \frac{G(r)}{r}$ which is bounded as $r \to 0$ and Eq.(16) becomes

$$G''(r) + \frac{1}{r^2}\left(-\varepsilon^2 r^2 - b^2 r - \ell(\ell+1)\right)G(r) = 0. \tag{21}$$

where $\varepsilon^2 = -\frac{2\mu E}{\hbar^2}$, $b^2 = -\frac{2\mu A}{\hbar^2}$ and $\lambda = \ell(\ell+1)$.

$$\tilde{\tau}(r) = 0, \quad \sigma(r) = r, \quad \tilde{\sigma}(r) = -\varepsilon^2 r^2 - b^2 r - \ell(\ell+1) \tag{22}$$

Using Eq.(9), $\pi(r)$ is found in four possible values as

$$\pi(r) = \frac{1}{2} \pm \begin{cases} (\sqrt{\varepsilon^2}\ r + \ell + \frac{1}{2}), & k_1 = -b^2 + 2\sqrt{\varepsilon^2}(\ell + \frac{1}{2}); \\ (\sqrt{\varepsilon^2}\ r - \ell - \frac{1}{2}), & k_2 = -b^2 - 2\sqrt{\varepsilon^2}(\ell + \frac{1}{2}). \end{cases} \tag{23}$$

where $k_{1,2}$ is determined by means of the same procedure as in [15]. From Eq.(6) we obtain

$$\tau(r) = \begin{cases} 1 + 2(\sqrt{\varepsilon^2}r + \ell + \frac{1}{2}), & k_1 = -b^2 + 2\sqrt{\varepsilon^2}(\ell + \frac{1}{2}), \\ 1 - 2(\sqrt{\varepsilon^2}r + \ell + \frac{1}{2}), & k_1 = -b^2 + 2\sqrt{\varepsilon^2}(\ell + \frac{1}{2}), \\ 1 + 2(\sqrt{\varepsilon^2}r + \ell + \frac{1}{2}), & k_1 = -b^2 - 2\sqrt{\varepsilon^2}(\ell + \frac{1}{2}), \\ 1 - 2(\sqrt{\varepsilon^2}r - \ell - \frac{1}{2}), & k_2 = -b^2 - 2\sqrt{\varepsilon^2}(\ell + \frac{1}{2}). \end{cases} \tag{24}$$

Imposing $\tau'(r) < 0$ [15], for $k_2 = -b^2 - 2\sqrt{\varepsilon^2}(\ell + \frac{1}{2})$ we obtain energy eigenvalues as

$$E_{n_1,\ell} = -\frac{\mu A^2}{2\hbar^2}\frac{1}{(n_1 + \ell + 1)^2} \tag{25}$$

which agrees with the results [5]. Following the same steps, we find the weight function as

$$\rho(s) = r^{2\ell+1}e^{-\sqrt{\varepsilon^2}r} \tag{26}$$

y_{n_1} is obtained by using Eq.(10)

$$y_{n_1,\ell}(r) = L_{n_1}^{(2\ell+1)}(r) \tag{27}$$

and also other part of the wave function

$$\phi(r) = r^{\ell+1}e^{-\sqrt{\varepsilon^2}r} \tag{28}$$

finally, the radial part solution is obtained as

$$G_{n_1,\ell}(r) = A_{n_1,\ell}\ r^{2\ell+1}e^{-\sqrt{\varepsilon^2}r}L_{n_1}^{2\ell+1}(r) \tag{29}$$

where $A_{n,\ell}$ is a normalization constant

$$A_{n_1,\ell} = \sqrt{\frac{n_1!}{2(n_1 + 2\ell + 1)(n_1 + 2\ell + 1)!}}$$

Hence, these radial solutions are consistent with refs.[5,17].

Now we solve angular part of the Schrödinger equation given in Eq.(17). Defining a new variable as

$$x = \cos\theta \tag{30}$$

then, Eq.(17) takes the form

$$\Theta''(x) - \frac{2x}{1 - x^2}\Theta' + \frac{1}{1 - x^2}^2\left(\lambda(1 - x^2) - (m^2 + \beta)\right)\Theta(x) = 0 \tag{31}$$

To apply the NU method, we define the polynomials

$$\tilde{\tau} = -2x,\ \ \sigma = 1 - x^2,\ \ \tilde{\sigma} = -\lambda x^2 + (\lambda - m^2 - \beta) \tag{32}$$

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where $\beta = \frac{2\mu B}{\hbar^2}$ and $\pi(x)$ becomes

$$\pi(x) = \pm \begin{cases} (\sqrt{m^2 + \beta}, & k_1 = \lambda; \\ (\sqrt{(m^2 + \beta)} \ x, & k_2 = \lambda - m^2 - \beta. \end{cases} \tag{33}$$

where $k_{1,2}$ is determined by means of the same procedure as in [15]. We obtain τ as

$$\tau(x) = \begin{cases} -2x + 2\sqrt{\beta + m^2}, & k_1 = \lambda, \\ -2x - 2\sqrt{\beta + m^2}, & k_1 = \lambda, \\ -2x + 2\sqrt{\beta + m^2}x, & k_2 = \lambda - m^2 - \beta, \\ -2x - 2\sqrt{\beta + m^2}x, & k_2 = \lambda - m^2 - \beta. \end{cases} \tag{34}$$

We impose $\tau'(x) < 0$ because of the physical solutions. For $k_2 = \lambda - m^2 - \beta$, we use negative sign of π in this case. Thus we obtain

$$\ell = n_2 + \sqrt{m^2 + \beta} \tag{35}$$

where we use $\lambda = \ell(\ell + 1)$. In order to get the wave function of the polar angle of Schrödinger equation, we use Eqs.(3) and (10-12) and one obtains,

$$\phi = (1 - x^2)^{\frac{1}{2}\sqrt{m^2 + \beta}} \tag{36}$$

and

$$\rho = (1 - x^2)^{-\sqrt{m^2 + \beta}} \tag{37}$$

$$y_n = B_n (1 - x^2)^{\sqrt{m^2 + \beta}} \frac{d^n}{dx^n} ((1 - x^2)^{n - \sqrt{m^2 + \beta}}) \tag{38}$$

where B_n is a normalization constant and the wave function is given as

$$\Theta_{n_2, \ell}(\theta) = C_{n_2} (\sin \theta)^{m'} P_{n_2}^{(m', m')}(\cos \theta) \tag{39}$$

where $m' = \sqrt{m^2 + \beta}$ and C_{n_2} is a normalization constant. Eq.(39) agrees with the results [5]. C_{n_2} is given as:

$$C_{n_2} = \sqrt{\frac{(2n_2 + 2m' + 1)\Gamma(n_2 + 1)\Gamma(n_2 + 2m' + 1)}{2^{2m' + 1}\Gamma(2n_2 + m' + 1)\Gamma(n_2 + m' + 1)}}$$

Therefore, the total energy of the system in Eq.(13) is given as (in a.u: $\mu = e = \hbar = 1, a_0 = 1, \epsilon_0 = -1/2$)

$$E_{(n_1,n_2),m} = -\frac{\eta^2 \sigma^4}{2(\sqrt{m^2 + \beta} + n_1 + n_2 + 1)^2} \tag{40}$$

which compares with ref.[1].

4 Conclusions

We have solved Schrödinger equation for the ring shaped potential. The energy eigenvalues and the corresponding eigenfunctions are obtained exactly by using NU-method. Eigenfunctions are expressed in terms of Laguerre and Jacobi polynomials for radial and angular parts respectively. It is seen that NU method is an applicable tool for not only central potentials but also noncentral and combined potentials. Results are in good agreement with the earlier works [1,5,6]. Some numerical results are given in Table 1. It is pointed out that for the values of $B = 0$, the results are in good agreement with ref. [6,25].

5 Acknowledgements

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Table 1: Energy levels for $\eta\sigma^2 = Z$, $\eta = 1$

n_1	n_2	m	E
1	1	0	-0.849763
2	2	0	-0.377661
		1	-0.330452
3	3	2	-0.178302
		1	-0.192028
		0	-0.212431
4	4	3	-0.112357
		2	-0.118038
		1	-0.125353
		0	-0.135954
5	5	4	-0.0776005
		3	-0.0804445
		2	-0.0838663
		1	-0.0882161
		0	-0.0944122